

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 3.79

Global applicability domain: Inside

Local applicability domain index: 9.86e-01

Confidence level: 7.64e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Anisole</div> <div>Measured: 4.01</div> <div>Predicted: 3.76</div>	<div>Image not found</div> <div>Pentyl acetate</div> <div>Measured: 4.12</div> <div>Predicted: 3.95</div>	<div>Image not found</div> <div>Chlorobenzene</div> <div>Measured: 3.31</div> <div>Predicted: 3.63</div>
<div>Image not found</div> <div>Octane</div> <div>Measured: 3.35</div> <div>Predicted: 3.62</div>	<div>Image not found</div> <div>2-Heptanone</div> <div>Measured: 4.15</div> <div>Predicted: 3.95</div>	